

# Study guide: Finite difference methods for wave motion

Hans Petter Langtangen<sup>1</sup>

Center for Biomedical Computing, Simula Research Laboratory and Department of Informatics, University of Oslo<sup>1</sup>

Sep 22, 2014

# 1 Finite difference methods for waves on a string

2 Verification

3 Implementation

- Making a solver function (3)

4 Vectorization

5 Generalization: reflecting boundaries

6 Generalization: variable wave velocity

7 Building a general 1D wave equation solver

8 Finite difference methods for 2D and 3D wave equations

9 Implementation of 2D/3D problems

10 Migrating loops to Cython

11 Migrating loops to Fortran

12 Migrating loops to C via Cython

13 Migrating loops to C via f2py

14 Analysis of the difference equations

Waves on a string can be modeled by the *wave equation*

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

$u(x, t)$  is the displacement of the string

Demo of waves on a string.

# The complete initial-boundary value problem

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L), \quad t \in (0, T] \quad (1)$$

$$u(x, 0) = l(x), \quad x \in [0, L] \quad (2)$$

$$\frac{\partial}{\partial t} u(x, 0) = 0, \quad x \in [0, L] \quad (3)$$

$$u(0, t) = 0, \quad t \in (0, T] \quad (4)$$

$$u(L, t) = 0, \quad t \in (0, T] \quad (5)$$

# Input data in the problem

- Initial condition  $u(x, 0) = l(x)$ : initial string shape
- Initial condition  $u_t(x, 0) = 0$ : string starts from rest
- $c = \sqrt{T/\varrho}$ : velocity of waves on the string
- ( $T$  is the tension in the string,  $\varrho$  is density of the string)
- Two boundary conditions on  $u$ :  $u = 0$  means fixed ends (no displacement)

Rule for number of initial and boundary conditions:

- $u_{tt}$  in the PDE: two initial conditions, on  $u$  and  $u_t$
- $u_t$  (and no  $u_{tt}$ ) in the PDE: one initial conditions, on  $u$
- $u_{xx}$  in the PDE: one boundary condition on  $u$  at each boundary point

## Demo of a vibrating string ( $C = 0.8$ )

- Our numerical method is sometimes exact (!)
- Our numerical method is sometimes subject to serious non-physical effects

## Demo of a vibrating string ( $C = 1.0012$ )

Ooops!

## Step 1: Discretizing the domain

Mesh in time:

$$0 = t_0 < t_1 < t_2 < \cdots < t_{N_t-1} < t_{N_t} = T \quad (6)$$

Mesh in space:

$$0 = x_0 < x_1 < x_2 < \cdots < x_{N_x-1} < x_{N_x} = L \quad (7)$$

Uniform mesh with constant mesh spacings  $\Delta t$  and  $\Delta x$ :

$$x_i = i\Delta x, \quad i = 0, \dots, N_x, \quad t_n = n\Delta t, \quad n = 0, \dots, N_t \quad (8)$$



# The discrete solution

- The numerical solution is a mesh function:  $u_i^n \approx u_e(x_i, t_n)$
- Finite difference stencil (or scheme): equation for  $u_i^n$  involving neighboring space-time points



## Step 2: Fulfilling the equation at the mesh points

Let the PDE be satisfied at all *interior* mesh points:

$$\frac{\partial^2}{\partial t^2} u(x_i, t_n) = c^2 \frac{\partial^2}{\partial x^2} u(x_i, t_n), \quad (9)$$

for  $i = 1, \dots, N_x - 1$  and  $n = 1, \dots, N_t - 1$ .

For  $n = 0$  we have the initial conditions  $u = l(x)$  and  $u_t = 0$ , and at the boundaries  $i = 0, N_x$  we have the boundary condition  $u = 0$ .

## Step 3: Replacing derivatives by finite differences

Widely used finite difference formula for the second-order derivative:

$$\frac{\partial^2}{\partial t^2} u(x_i, t_n) \approx \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = [D_t D_t u]_i^n$$

and

$$\frac{\partial^2}{\partial x^2} u(x_i, t_n) \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} = [D_x D_x u]_i^n$$

## Step 3: Algebraic version of the PDE

Replace derivatives by differences:

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = c^2 \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}, \quad (10)$$

In operator notation:

$$[D_t D_t u = c^2 D_x D_x]_i^n \quad (11)$$

### Step 3: Algebraic version of the initial conditions

- Need to replace the derivative in the initial condition  $u_t(x, 0) = 0$  by a finite difference approximation
- The differences for  $u_{tt}$  and  $u_{xx}$  have second-order accuracy
- Use a centered difference for  $u_t(x, 0)$

$$[D_{2t}u]_i^n = 0, \quad n = 0 \quad \Rightarrow \quad u_i^{n-1} = u_i^{n+1}, \quad i = 0, \dots, N_x$$

The other initial condition  $u(x, 0) = I(x)$  can be computed by

$$u_i^0 = I(x_i), \quad i = 0, \dots, N_x$$

## Step 4: Formulating a recursive algorithm

- Nature of the algorithm: compute  $u$  in space at  $t = \Delta t, 2\Delta t, 3\Delta t, \dots$
- Three time levels are involved in the general discrete equation:  $n + 1, n, n - 1$
- $u_i^n$  and  $u_i^{n-1}$  are then already computed for  $i = 0, \dots, N_x$ , and  $u_i^{n+1}$  is the unknown quantity

Write out  $[D_t D_t u = c^2 D_x D_x]_i^n$  and solve for  $u_i^{n+1}$ ,

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2 (u_{i+1}^n - 2u_i^n + u_{i-1}^n) \quad (12)$$

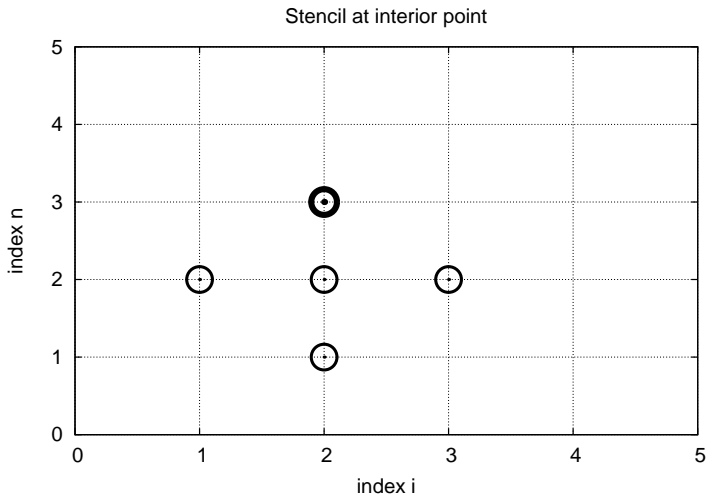
$$C = c \frac{\Delta t}{\Delta x}, \quad (13)$$

is known as the (dimensionless) *Courant number*

### Observe

There is only one parameter,  $C$ , in the discrete model:  $C$  lumps mesh parameters  $\Delta t$  and  $\Delta x$  with the only physical parameter, the wave velocity  $c$ . The value  $C$  and the smoothness of  $I(x)$  govern the quality of the numerical solution.

# The finite difference stencil





# The stencil for the first time level

- Problem: the stencil for  $n = 1$  involves  $u_i^{-1}$ , but time  $t = -\Delta t$  is outside the mesh
- Remedy: use the initial condition  $u_t = 0$  together with the stencil to eliminate  $u_i^{-1}$

Initial condition:

$$[D_{2t}u = 0]_i^0 \Rightarrow u_i^{-1} = u_i^1$$

Insert in stencil  $[D_t D_t u = c^2 D_x D_x]_i^0$  to get

$$u_i^1 = u_i^0 - \frac{1}{2} C^2 (u_{i+1}^n - 2u_i^n + u_{i-1}^n) \quad (14)$$

# The algorithm

- 1 Compute  $u_i^0 = I(x_i)$  for  $i = 0, \dots, N_x$
- 2 Compute  $u_i^1$  by (14) and set  $u_i^1 = 0$  for the boundary points  $i = 0$  and  $i = N_x$ , for  $n = 1, 2, \dots, N - 1$ ,
- 3 For each time level  $n = 1, 2, \dots, N_t - 1$ 
  - 1 apply (12) to find  $u_i^{n+1}$  for  $i = 1, \dots, N_x - 1$
  - 2 set  $u_i^{n+1} = 0$  for the boundary points  $i = 0, i = N_x$ .

# Moving finite difference stencil

web page or a movie file.

# Sketch of an implementation (1)

- Arrays:
  - $u[i]$  stores  $u_i^{n+1}$
  - $u\_1[i]$  stores  $u_i^n$
  - $u\_2[i]$  stores  $u_i^{n-1}$

## Naming convention

$u$  is the unknown to be computed (a spatial mesh function),  $u\_k$  is the computed spatial mesh function  $k$  time steps back in time.

# PDE solvers should save memory

## Important to minimize the memory usage

The algorithm only needs to access the *three most recent time levels*, so we need only three arrays for  $u_i^{n+1}$ ,  $u_i^n$ , and  $u_i^{n-1}$ ,  $i = 0, \dots, N_x$ . Storing all the solutions in a two-dimensional array of size  $(N_x + 1) \times (N_t + 1)$  would be possible in this simple one-dimensional PDE problem, but not in large 2D problems and not even in small 3D problems.

## Sketch of an implementation (2)

```
# Given mesh points as arrays x and t (x[i], t[n])
dx = x[1] - x[0]
dt = t[1] - t[0]
C = c*dt/dx          # Courant number
Nt = len(t)-1
C2 = C**2            # Help variable in the scheme

# Set initial condition u(x,0) = I(x)
for i in range(0, Nx+1):
    u_1[i] = I(x[i])

# Apply special formula for first step, incorporating du/dt=0
for i in range(1, Nx):
    u[i] = u_1[i] - 0.5*C**2(u_1[i+1] - 2*u_1[i] + u_1[i-1])
u[0] = 0; u[Nx] = 0    # Enforce boundary conditions

# Switch variables before next step
u_2[:,], u_1[:,] = u_1, u

for n in range(1, Nt):
    # Update all inner mesh points at time t[n+1]
    for i in range(1, Nx):
        u[i] = 2*u_1[i] - u_2[i] - \
            C**2(u_1[i+1] - 2*u_1[i] + u_1[i-1])

    # Insert boundary conditions
    u[0] = 0; u[Nx] = 0
```

1 Finite difference methods for waves on a string

2 **Verification**

3 Implementation

- Making a solver function (3)

4 Vectorization

5 Generalization: reflecting boundaries

6 Generalization: variable wave velocity

7 Building a general 1D wave equation solver

8 Finite difference methods for 2D and 3D wave equations

9 Implementation of 2D/3D problems

10 Migrating loops to Cython

11 Migrating loops to Fortran

12 Migrating loops to C via Cython

13 Migrating loops to C via f2py

14 Analysis of the difference equations

- Think about testing and verification before you start implementing the algorithm!
- Powerful testing tool: method of manufactured solutions and computation of convergence rates
- Will need a source term in the PDE and  $u_t(x, 0) \neq 0$
- Even more powerful method: exact solution of the scheme



## A slightly generalized model problem

Add source term  $f$  and nonzero initial condition  $u_t(x, 0)$ :

$$u_{tt} = c^2 u_{xx} + f(x, t), \quad (15)$$

$$u(x, 0) = I(x), \quad x \in [0, L] \quad (16)$$

$$u_t(x, 0) = V(x), \quad x \in [0, L] \quad (17)$$

$$u(0, t) = 0, \quad t > 0, \quad (18)$$

$$u(L, t) = 0, \quad t > 0 \quad (19)$$

$$[D_t D_t u = c^2 D_x D_x + f]_i^n \quad (20)$$

Writing out and solving for the unknown  $u_i^{n+1}$ :

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + \Delta t^2 f_i^n \quad (21)$$

## Modified equation for the first time level

Centered difference for  $u_t(x, 0) = V(x)$ :

$$[D_{2t}u = V]_i^0 \Rightarrow u_i^{-1} = u_i^1 - 2\Delta t V_i,$$

Inserting this in the stencil (21) for  $n = 0$  leads to

$$u_i^1 = u_i^0 - \Delta t V_i + \frac{1}{2}C^2 (u_{i+1}^n - 2u_i^n + u_{i-1}^n) + \frac{1}{2}\Delta t^2 f_i^n \quad (22)$$

## Using an analytical solution of physical significance

- Standing waves occur in real life on a string
- Can be analyzed mathematically (known exact solution)

$$u_e(x, y, t) = A \sin\left(\frac{\pi}{L}x\right) \cos\left(\frac{\pi}{L}ct\right) \quad (23)$$

- PDE data:  $f = 0$ , boundary conditions  $u_e(0, t) = u_e(L, 0) = 0$ , initial conditions  $l(x) = A \sin\left(\frac{\pi}{L}x\right)$  and  $V = 0$
- Note:  $u_i^{n+1} \neq u_e(x_i, t_{n+1})$ , and we do not know the error, so testing must aim at reproducing the expected convergence rates

# Manufactured solution: principles

- Disadvantage with the previous physical solution: it does not test  $V \neq 0$  and  $f \neq 0$
- Method of manufactured solution:
  - Choose some  $u_e(x, t)$
  - Insert in PDE and fit  $f$
  - Set boundary and initial conditions compatible with the chosen  $u_e(x, t)$

## Manufactured solution: example

$$u_e(x, t) = x(L - x) \sin t$$

PDE  $u_{tt} = c^2 u_{xx} + f$ :

$$-x(L - x) \sin t = -2 \sin t + f \quad \Rightarrow f = (2 - x(L - x)) \sin t$$

Initial conditions become

$$u(x, 0) = I(x) = 0$$

$$u_t(x, 0) = V(x) = (2 - x(L - x)) \cos t$$

Boundary conditions:

$$u(x, 0) = u(x, L) = 0$$

# Testing a manufactured solution

- Introduce common mesh parameter:  $h = \Delta t$ ,  $\Delta x = ch/C$
- This  $h$  keeps  $C$  and  $\Delta t/\Delta x$  constant
- Select coarse mesh  $h$ :  $h_0$
- Run experiments with  $h_i = 2^{-i}h_0$  (halving the cell size),  
 $i = 0, \dots, m$
- Record the error  $E_i$  and  $h_i$  in each experiment
- Compute pairwise convergence rates  $r_i = \ln E_{i+1}/E_i / \ln h_{i+1}/h_i$
- Verification:  $r_i \rightarrow 2$  as  $i$  increases

# Constructing an exact solution of the discrete equations

- Manufactured solution with computation of convergence rates: much manual work
- Simpler and more powerful: use an exact solution for  $u_i^n$
- A linear or quadratic  $u_e$  in  $x$  and  $t$  is often a good candidate



## Analytical work with the PDE problem

Here, choose  $u_e$  such that  $u_e(x, 0) = u_e(L, 0) = 0$ :

$$u_e(x, t) = x(L - x)\left(1 + \frac{1}{2}t\right),$$

Insert in the PDE and find  $f$ :

$$f(x, t) = 2(1 + t)c^2$$

Initial conditions:

$$I(x) = x(L - x), \quad V(x) = \frac{1}{2}x(L - x)$$

# Analytical work with the discrete equations (1)

We want to show that  $u_e$  also solves the discrete equations!

Useful preliminary result:

$$[D_t D_t t^2]^n = \frac{t_{n+1}^2 - 2t_n^2 + t_{n-1}^2}{\Delta t^2} = (n+1)^2 - n^2 + (n-1)^2 = 2 \quad (24)$$

$$[D_t D_t t]^n = \frac{t_{n+1} - 2t_n + t_{n-1}}{\Delta t^2} = \frac{((n+1) - n + (n-1))\Delta t}{\Delta t^2} = 0 \quad (25)$$

Hence,

$$[D_t D_t u_e]_i^n = x_i(L - x_i)[D_t D_t (1 + \frac{1}{2}t)]^n = x_i(L - x_i)\frac{1}{2}[D_t D_t t]^n = 0$$

## Analytical work with the discrete equations (1)

$$\begin{aligned}[D_x D_x u_e]_i^n &= (1 + \frac{1}{2}t_n)[D_x D_x (xL - x^2)]_i = (1 + \frac{1}{2}t_n)[LD_x D_x x - D_x D_x x^2] \\ &= -2(1 + \frac{1}{2}t_n)\end{aligned}$$

Now,  $f_i^n = 2(1 + \frac{1}{2}t_n)c^2$  and we get

$$[D_t D_t u_e - c^2 D_x D_x u_e - f]_i^n = 0 - c^2(-1)2(1 + \frac{1}{2}t_n) + 2(1 + \frac{1}{2}t_n)c^2 = 0$$

Moreover,  $u_e(x_i, 0) = I(x_i)$ ,  $\partial u_e / \partial t = V(x_i)$  at  $t = 0$ , and  $u_e(x_0, t) = u_e(x_{N_x}, 0) = 0$ . Also the modified scheme for the first time step is fulfilled by  $u_e(x_i, t_n)$ .

# Testing with the exact discrete solution

- We have established that
$$u_i^{n+1} = u_e(x_i, t_{n+1}) = x_i(L - x_i)(1 + t_{n+1}/2)$$
- Run *one* simulation with one choice of  $c$ ,  $\Delta t$ , and  $\Delta x$
- Check that  $\max_i |u_i^{n+1} - u_e(x_i, t_{n+1})| < \epsilon$ ,  $\epsilon \sim 10^{-14}$  (machine precision + some round-off errors)
- This is the simplest and best verification test

Later we show that the exact solution of the discrete equations can be obtained by  $C = 1$  (!)

## Testing with the exact discrete solution

- We have established that
$$u_i^{n+1} = u_e(x_i, t_{n+1}) = x_i(L - x_i)(1 + t_{n+1}/2)$$
- Run *one* simulation with one choice of  $c$ ,  $\Delta t$ , and  $\Delta x$
- Check that  $\max_i |u_i^{n+1} - u_e(x_i, t_{n+1})| < \epsilon$ ,  $\epsilon \sim 10^{-14}$  (machine precision + some round-off errors)
- This is the simplest and best verification test

Later we show that the exact solution of the discrete equations can be obtained by  $C = 1$  (!)

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 **Implementation**
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

# The algorithm

- ➊ Compute  $u_i^0 = I(x_i)$  for  $i = 0, \dots, N_x$
- ➋ Compute  $u_i^1$  by (14) and set  $u_i^1 = 0$  for the boundary points  $i = 0$  and  $i = N_x$ , for  $n = 1, 2, \dots, N - 1$ ,
- ➌ For each time level  $n = 1, 2, \dots, N_t - 1$ 
  - ➊ apply (12) to find  $u_i^{n+1}$  for  $i = 1, \dots, N_x - 1$
  - ➋ set  $u_i^{n+1} = 0$  for the boundary points  $i = 0, i = N_x$ .

# What do to with the solution?

- Different problem settings demand different actions with the computed  $u_i^{n+1}$  at each time step
- Solution: let the solver function make a callback to a user function where the user can do whatever is desired with the solution
- Advantage: solver just solves and user uses the solution

```
def user_action(u, x, t, n):  
    # u[i] at spatial mesh points x[i] at time t[n]  
    # plot u  
    # or store u
```



# Making a solver function (1)

We specify  $\Delta t$  and  $C$ , and let the solver function compute  $\Delta x = c\Delta t/C$ .

```
def solver(I, V, f, c, L, dt, C, T, user_action=None):
    """Solve  $u_{tt} = c^2 u_{xx} + f$  on  $(0, L) \times (0, T]$ ."""
    Nt = int(round(T/dt))
    t = linspace(0, Nt*dt, Nt+1)    # Mesh points in time
    dx = dt*c/float(C)
    Nx = int(round(L/dx))
    x = linspace(0, L, Nx+1)        # Mesh points in space
    dx = x[1] - x[0]
    C2 = C**2                        # Help variable in the scheme

    if f is None or f == 0 :
        f = lambda x, t: 0
    if V is None or V == 0:
        V = lambda x: 0

    u    = zeros(Nx+1)    # Solution array at new time level
    u_1  = zeros(Nx+1)    # Solution at 1 time level back
    u_2  = zeros(Nx+1)    # Solution at 2 time levels back

    import time; t0 = time.clock() # for measuring CPU time

    # Load initial condition into u_1
    for i in range(0, Nx+1):
        u_1[i] = I(x[i])
```

## Making a solver function (2)

```
def solver(I, V, f, c, L, dt, C, T, user_action=None):
    ...
    # Special formula for first time step
    n = 0
    for i in range(1, Nx):
        u[i] = u_1[i] + dt*V(x[i]) + \
            0.5*C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1]) + \
            0.5*dt**2*f(x[i], t[n])
    u[0] = 0; u[Nx] = 0

    if user_action is not None:
        user_action(u, x, t, 1)

    # Switch variables before next step
    u_2[:, u_1[:]] = u_1, u

def solver(I, V, f, c, L, Nx, C, T, user_action=None):
    ...
    # Time loop

    for n in range(1, Nt):
        # Update all inner points at time t[n+1]
        for i in range(1, Nx):
            u[i] = - u_2[i] + 2*u_1[i] + \
                C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1]) + \
                dt**2*f(x[i], t[n])
```

## Verification: exact quadratic solution

Exact solution of the PDE problem *and* the discrete equations:

$$u_e(x, t) = x(L - x)(1 + \frac{1}{2}t)$$

```
import nose.tools as nt

def test_quadratic():
    """Check that u(x, t)=x(L-x)(1+t/2) is exactly reproduced."""
    def u_exact(x, t):
        return x*(L-x)*(1 + 0.5*t)

    def I(x):
        return u_exact(x, 0)

    def V(x):
        return 0.5*u_exact(x, 0)

    def f(x, t):
        return 2*(1 + 0.5*t)*c**2

    L = 2.5
    c = 1.5
    C = 0.75
    Nx = 3 # Very coarse mesh for this exact test
    dt = C*(L/Nx)/c
    T = 18

    u, x, t, cpu = solver(I, V, f, c, L, dt, C, T)
```

## Visualization: animating $u(x, t)$

Make a viz function for animating the curve, with plotting in a user\_action function plot\_u:

```
def viz(I, V, f, c, L, dt, C, T, umin, umax, animate=True):
    """Run solver and visualize u at each time level."""
    import scitools.std as plt
    import time, glob, os

    def plot_u(u, x, t, n):
        """user_action function for solver."""
        plt.plot(x, u, 'r-',
                 xlabel='x', ylabel='u',
                 axis=[0, L, umin, umax],
                 title='t=%f' % t[n], show=True)
        # Let the initial condition stay on the screen for 2
        # seconds, else insert a pause of 0.2 s between each plot
        time.sleep(2) if t[n] == 0 else time.sleep(0.2)
        plt.savefig('frame_%04d.png' % n) # for movie making

    # Clean up old movie frames
    for filename in glob.glob('frame_*.png'):
        os.remove(filename)

    user_action = plot_u if animate else None
    u, x, t, cpu = solver(I, V, f, c, L, dt, C, T, user_action)

    # Make movie files
```

# Making movie files

- Store spatial curve in a file, for each time level
- Name files like 'something\_%04d.png' % frame\_counter
- Combine files to a movie

```
Terminal> scitools movie encoder=html output_file=movie.html \
          fps=4 frame_*.png # web page with a player
Terminal> avconv -r 4 -i frame_%04d.png -c:v flv          movie.flv
Terminal> avconv -r 4 -i frame_%04d.png -c:v libtheora movie.ogg
Terminal> avconv -r 4 -i frame_%04d.png -c:v libx264      movie.mp4
Terminal> avconv -r 4 -i frame_%04d.png -c:v libpx      movie.webm
```

## Important

- Zero padding (%04d) is essential for correct sequence of frames in something\_\*.png (Unix alphanumeric sort)
- Remove old frame\_\*.png files before making a new movie

- Vibrations of a guitar string
- Triangular initial shape (at rest)

$$I(x) = \begin{cases} ax/x_0, & x < x_0 \\ a(L-x)/(L-x_0), & \text{otherwise} \end{cases} \quad (26)$$

Appropriate data:

- $L = 75$  cm,  $x_0 = 0.8L$ ,  $a = 5$  mm, time frequency  $\nu = 440$  Hz

# Implementation of the case

```
def guitar(C):  
    """Triangular wave (pulled guitar string)."""  
    L = 0.75  
    x0 = 0.8*L  
    a = 0.005  
    freq = 440  
    wavelength = 2*L  
    c = freq*wavelength  
    omega = 2*pi*freq  
    num_periods = 1  
    T = 2*pi/omega*num_periods  
    # Choose dt the same as the stability limit for Nx=50  
    dt = L/50./c  
  
    def I(x):  
        return a*x/x0 if x < x0 else a/(L-x0)*(L-x)  
  
    umin = -1.2*a;    umax = -umin  
    cpu = viz(I, 0, 0, c, L, dt, C, T, umin, umax, animate=True)
```

Program: `wave1D_u0.py`.

## Resulting movie for $C = 0.8$

Movie of the vibrating string



# The benefits of scaling

- It is difficult to figure out all the physical parameters of a case
- And it is not necessary because of a powerful: *scaling*

Introduce new  $x$ ,  $t$ , and  $u$  without dimension:

$$\bar{x} = \frac{x}{L}, \quad \bar{t} = \frac{c}{L}t, \quad \bar{u} = \frac{u}{a}$$

Insert this in the PDE (with  $f = 0$ ) and dropping bars

$$u_{tt} = u_{xx}$$

Initial condition: set  $a = 1$ ,  $L = 1$ , and  $x_0 \in [0, 1]$  in (26).

In the code: set  $a=c=L=1$ ,  $x_0=0.8$ , and there is no need to calculate with wavelengths and frequencies to estimate  $c$ !

Just one challenge: determine the period of the waves and an appropriate end time (see the text for details).

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization**
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

- Problem: Python loops over long arrays are slow
- One remedy: use vectorized (numpy) code instead of explicit loops
- Other remedies: use Cython, port spatial loops to Fortran or C
- Speedup: 100-1000 (varies with  $N_x$ )

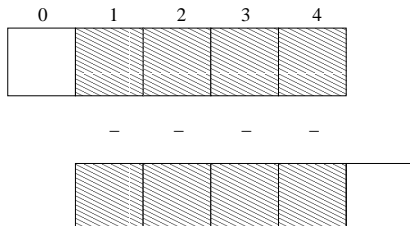
Next: vectorized loops

# Operations on slices of arrays

- Introductory example: compute  $d_i = u_{i+1} - u_i$

```
n = u.size
for i in range(0, n-1):
    d[i] = u[i+1] - u[i]
```

- Note: all the differences here are independent of each other.
- Therefore  $d = (u_1, u_2, \dots, u_n) - (u_0, u_1, \dots, u_{n-1})$
- In numpy code: `u[1:n] - u[0:n-1]` or just `u[1:] - u[:-1]`



# Test the understanding

Newcomers to vectorization are encouraged to choose a small array  $u$ , say with five elements, and simulate with pen and paper both the loop version and the vectorized version.

# Vectorization of finite difference schemes (1)

Finite difference schemes basically contains differences between array elements with shifted indices. Consider the updating formula

```
for i in range(1, n-1):  
    u2[i] = u[i-1] - 2*u[i] + u[i+1]
```

The vectorization consists of replacing the loop by arithmetics on slices of arrays of length  $n-2$ :

```
u2 = u[:-2] - 2*u[1:-1] + u[2:]  
u2 = u[0:n-2] - 2*u[1:n-1] + u[2:n]    # alternative
```

Note:  $u_2$  gets length  $n-2$ .

If  $u_2$  is already an array of length  $n$ , do update on "inner" elements

```
u2[1:-1] = u[:-2] - 2*u[1:-1] + u[2:]  
u2[1:n-1] = u[0:n-2] - 2*u[1:n-1] + u[2:n]    # alternative
```

## Vectorization of finite difference schemes (2)

Include a function evaluation too:

```
def f(x):  
    return x**2 + 1  
  
# Scalar version  
for i in range(1, n-1):  
    u2[i] = u[i-1] - 2*u[i] + u[i+1] + f(x[i])  
  
# Vectorized version  
u2[1:-1] = u[:-2] - 2*u[1:-1] + u[2:] + f(x[1:-1])
```

# Vectorized implementation in the solver function

Scalar loop:

```
for i in range(1, Nx):  
    u[i] = 2*u_1[i] - u_2[i] + \  
          C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
```

Vectorized loop:

```
u[1:-1] = - u_2[1:-1] + 2*u_1[1:-1] + \  
          C2*(u_1[:-2] - 2*u_1[1:-1] + u_1[2:])
```

or

```
u[1:Nx] = 2*u_1[1:Nx] - u_2[1:Nx] + \  
          C2*(u_1[0:Nx-1] - 2*u_1[1:Nx] + u_1[2:Nx+1])
```

Program: [wave1D\\_u0v.py](#)



# Verification of the vectorized version

```
def test_quadratic():  
    """  
    Check the scalar and vectorized versions work for  
    a quadratic  $u(x,t)=x(L-x)(1+t/2)$  that is exactly reproduced.  
    """  
    # The following function must work for x as array or scalar  
    u_exact = lambda x, t: x*(L - x)*(1 + 0.5*t)  
    I = lambda x: u_exact(x, 0)  
    V = lambda x: 0.5*u_exact(x, 0)  
    # f is a scalar (zeros_like(x) works for scalar x too)  
    f = lambda x, t: zeros_like(x) + 2*c**2*(1 + 0.5*t)  
  
    L = 2.5  
    c = 1.5  
    C = 0.75  
    Nx = 3 # Very coarse mesh for this exact test  
    dt = C*(L/Nx)/c  
    T = 18  
  
    def assert_no_error(u, x, t, n):  
        u_e = u_exact(x, t[n])  
        diff = abs(u - u_e).max()  
        nt.assert_almost_equal(diff, 0, places=13)  
  
    solver(I, V, f, c, L, dt, C, T,  
           user_action=assert_no_error, version='scalar')  
    solver(I, V, f, c, L, dt, C, T,  
           user_action=assert_no_error, version='vectorized')
```

- Run `wave1D_u0v.py` for  $N_x$  as 50,100,200,400,800 and measuring the CPU time
- Observe substantial speed-up: vectorized version is about  $N_x/5$  times faster

Much bigger improvements for 2D and 3D codes!

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries**
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

- Boundary condition  $u = 0$ :  $u$  changes sign
- Boundary condition  $u_x = 0$ : wave is perfectly reflected
- How can we implement  $u_x$ ? (more complicated than  $u = 0$ )

Demo of boundary conditions

$$\frac{\partial u}{\partial n} \equiv \mathbf{n} \cdot \nabla u = 0 \quad (27)$$

For a 1D domain  $[0, L]$ :

$$\left. \frac{\partial}{\partial n} \right|_{x=L} = \frac{\partial}{\partial x}, \quad \left. \frac{\partial}{\partial n} \right|_{x=0} = -\frac{\partial}{\partial x}$$

Boundary condition terminology:

- $u_x$  specified: **Neumann** condition
- $u$  specified: **Dirichlet** condition

## Discretization of derivatives at the boundary (1)

- How can we incorporate the condition  $u_x = 0$  in the finite difference scheme?
- We used central differences for  $u_{tt}$  and  $u_{xx}$ :  $\mathcal{O}(\Delta t^2, \Delta x^2)$  accuracy
- Also for  $u_t(x, 0)$
- Should use central difference for  $u_x$  to preserve second order accuracy

$$\frac{u_{-1}^n - u_1^n}{2\Delta x} = 0 \quad (28)$$

## Discretization of derivatives at the boundary (2)

$$\frac{u_{-1}^n - u_1^n}{2\Delta x} = 0$$

- Problem:  $u_{-1}^n$  is outside the mesh (fictitious value)
- Remedy: use the stencil at the boundary to eliminate  $u_{-1}^n$ ; just replace  $u_{-1}^n$  by  $u_1^n$

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + 2C^2 (u_{i+1}^n - u_i^n), \quad i = 0 \quad (29)$$

# Visualization of modified boundary stencil

Discrete equation for computing  $u_0^3$  in terms of  $u_0^2$ ,  $u_0^1$ , and  $u_1^2$ :

Animation in a [web page](#) or a [movie file](#).



# Implementation of Neumann conditions

- Use the general stencil for interior points also on the boundary
- Replace  $u_{i-1}^n$  by  $u_{i+1}^n$  for  $i = 0$
- Replace  $u_{i+1}^n$  by  $u_{i-1}^n$  for  $i = N_x$

```
i = 0
ip1 = i+1
im1 = ip1 # i-1 -> i+1
u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])
```

```
i = Nx
im1 = i-1
ip1 = im1 # i+1 -> i-1
u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])
```

# Or just one loop over all points

```
for i in range(0, Nx+1):
    ip1 = i+1 if i < Nx else i-1
    im1 = i-1 if i > 0 else i+1
    u[i] = u_1[i] + C2*(u_1[im1] - 2*u_1[i] + u_1[ip1])
```

Program [wave1D\\_dn0.py](#)

# Moving finite difference stencil

web page or a movie file.

# Index set notation

- Tedious to write index sets like  $i = 0, \dots, N_x$  and  $n = 0, \dots, N_t$
- Notation not valid if  $i$  or  $n$  starts at 1 instead...
- Both in math and code it is advantageous to use *index sets*
- $i \in \mathcal{I}_x$  instead of  $i = 0, \dots, N_x$
- Definition:  $\mathcal{I}_x = \{0, \dots, N_x\}$
- The first index:  $i = \mathcal{I}_x^0$
- The last index:  $i = \mathcal{I}_x^{-1}$
- All interior points:  $i \in \mathcal{I}_x^i$ ,  $\mathcal{I}_x^i = \{1, \dots, N_x - 1\}$
- $\mathcal{I}_x^-$  means  $\{0, \dots, N_x - 1\}$
- $\mathcal{I}_x^+$  means  $\{1, \dots, N_x\}$

# Index set notation in code

Notation	Python
$\mathcal{I}_x$	<code>Ix</code>
$\mathcal{I}_x^0$	<code>Ix[0]</code>
$\mathcal{I}_x^{-1}$	<code>Ix[-1]</code>
$\mathcal{I}_x^-$	<code>Ix[1:]</code>
$\mathcal{I}_x^+$	<code>Ix[: -1]</code>
$\mathcal{I}_x^i$	<code>Ix[1: -1]</code>

## Index sets in action (1)

Index sets for a problem in the  $x, t$  plane:

$$\mathcal{I}_x = \{0, \dots, N_x\}, \quad \mathcal{I}_t = \{0, \dots, N_t\}, \quad (30)$$

Implemented in Python as

```
Ix = range(0, Nx+1)
It = range(0, Nt+1)
```

## Index sets in action (2)

A finite difference scheme can with the index set notation be specified as

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2 (u_{i+1}^n - 2u_i^n + u_{i-1}^n), \quad i \in \mathcal{I}_x^i, \quad n \in \mathcal{I}_t^i$$

$$u_i = 0, \quad i = \mathcal{I}_x^0, \quad n \in \mathcal{I}_t^i$$

$$u_i = 0, \quad i = \mathcal{I}_x^{-1}, \quad n \in \mathcal{I}_t^i$$

Corresponding implementation:

```
for n in It[1:-1]:
    for i in Ix[1:-1]:
        u[i] = - u_2[i] + 2*u_1[i] + \
                C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
    i = Ix[0]; u[i] = 0
    i = Ix[-1]; u[i] = 0
```

Program `wave1D_dn.py`

## Alternative implementation via ghost cells

- Instead of modifying the stencil at the boundary, we extend the mesh to cover  $u_{-1}^n$  and  $u_{N_x+1}^n$
- The extra left and right cell are called *ghost cells*
- The extra points are called *ghost points*
- The  $u_{-1}^n$  and  $u_{N_x+1}^n$  values are called *ghost values*
- Update ghost values as  $u_{i-1}^n = u_{i+1}^n$  for  $i = 0$  and  $i = N_x$
- Then the stencil becomes right at the boundary

# Implementation of ghost cells (1)

Add ghost points:

```
u    = zeros(Nx+3)
u_1  = zeros(Nx+3)
u_2  = zeros(Nx+3)

x = linspace(0, L, Nx+1)  # Mesh points without ghost points
```

- A major indexing problem arises with ghost cells since Python indices *must* start at 0.
- `u[-1]` will always mean the last element in `u`
- Math indexing:  $-1, 0, 1, 2, \dots, N_x + 1$
- Python indexing:  $0, \dots, Nx+2$
- Remedy: use index sets



## Implementation of ghost cells (2)

```
u = zeros(Nx+3)
Ix = range(1, u.shape[0]-1)

# Boundary values: u[Ix[0]], u[Ix[-1]]

# Set initial conditions
for i in Ix:
    u_1[i] = I(x[i-Ix[0]]) # Note i-Ix[0]

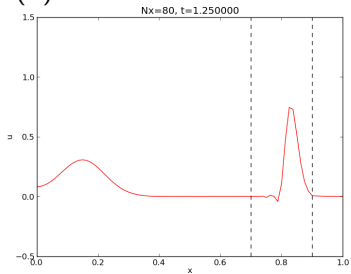
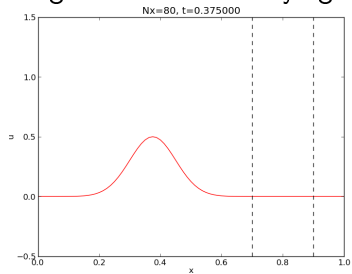
# Loop over all physical mesh points
for i in Ix:
    u[i] = - u_2[i] + 2*u_1[i] + \
           C2*(u_1[i-1] - 2*u_1[i] + u_1[i+1])

# Update ghost values
i = Ix[0] # x=0 boundary
u[i-1] = u[i+1]
i = Ix[-1] # x=L boundary
u[i-1] = u[i+1]
```

Program: `wave1D_dn0_ghost.py`.

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity**
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

## Heterogeneous media: varying $c = c(x)$



$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right) + f(x, t) \quad (31)$$

This equation sampled at a mesh point  $(x_i, t_n)$ :

$$\frac{\partial^2}{\partial t^2} u(x_i, t_n) = \frac{\partial}{\partial x} \left( q(x_i) \frac{\partial}{\partial x} u(x_i, t_n) \right) + f(x_i, t_n),$$

## Discretizing the variable coefficient (1)

The principal idea is to *first discretize the outer derivative*.

Define

$$\phi = q(x) \frac{\partial u}{\partial x}$$

Then use a centered derivative around  $x = x_i$  for the derivative of  $\phi$ :

$$\left[ \frac{\partial \phi}{\partial x} \right]_i^n \approx \frac{\phi_{i+\frac{1}{2}} - \phi_{i-\frac{1}{2}}}{\Delta x} = [D_x \phi]_i^n$$

## Discretizing the variable coefficient (2)

Then discretize the inner operators:

$$\phi_{i+\frac{1}{2}} = q_{i+\frac{1}{2}} \left[ \frac{\partial u}{\partial x} \right]_{i+\frac{1}{2}}^n \approx q_{i+\frac{1}{2}} \frac{u_{i+1}^n - u_i^n}{\Delta x} = [q D_x u]_{i+\frac{1}{2}}^n$$

Similarly,

$$\phi_{i-\frac{1}{2}} = q_{i-\frac{1}{2}} \left[ \frac{\partial u}{\partial x} \right]_{i-\frac{1}{2}}^n \approx q_{i-\frac{1}{2}} \frac{u_i^n - u_{i-1}^n}{\Delta x} = [q D_x u]_{i-\frac{1}{2}}^n$$

## Discretizing the variable coefficient (3)

These intermediate results are now combined to

$$\left[ \frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right) \right]_i^n \approx \frac{1}{\Delta x^2} \left( q_{i+\frac{1}{2}} (u_{i+1}^n - u_i^n) - q_{i-\frac{1}{2}} (u_i^n - u_{i-1}^n) \right) \quad (32)$$

In operator notation:

$$\left[ \frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right) \right]_i^n \approx [D_x q D_x u]_i^n \quad (33)$$

### Remark

Many are tempted to use the chain rule on the term  $\frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right)$ , but this is not a good idea!

# Computing the coefficient between mesh points

- Given  $q(x)$ : compute  $q_{i+\frac{1}{2}}$  as  $q(x_{i+\frac{1}{2}})$
- Given  $q$  at the mesh points:  $q_i$ , use an average

$$q_{i+\frac{1}{2}} \approx \frac{1}{2} (q_i + q_{i+1}) = [\bar{q}^x]_i \quad (\text{arithmetic mean}) \quad (34)$$

$$q_{i+\frac{1}{2}} \approx 2 \left( \frac{1}{q_i} + \frac{1}{q_{i+1}} \right)^{-1} \quad (\text{harmonic mean}) \quad (35)$$

$$q_{i+\frac{1}{2}} \approx (q_i q_{i+1})^{1/2} \quad (\text{geometric mean}) \quad (36)$$

The arithmetic mean in (34) is by far the most used averaging technique.



## Discretization of variable-coefficient wave equation in operator notation

$$[D_t D_t u = D_x \bar{q}^x D_x u + f]_i^n \quad (37)$$

We clearly see the type of finite differences and averaging!

Write out and solve wrt  $u_i^{n+1}$ :

$$\begin{aligned} u_i^{n+1} = & -u_i^{n-1} + 2u_i^n + \left(\frac{\Delta x}{\Delta t}\right)^2 \times \\ & \left( \frac{1}{2}(q_i + q_{i+1})(u_{i+1}^n - u_i^n) - \frac{1}{2}(q_i + q_{i-1})(u_i^n - u_{i-1}^n) \right) + \\ & \Delta t^2 f_i^n \end{aligned} \quad (38)$$

## Neumann condition and a variable coefficient

Consider  $\partial u / \partial x = 0$  at  $x = L = N_x \Delta x$ :

$$\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = 0 \quad u_{i+1}^n = u_{i-1}^n, \quad i = N_x$$

Insert  $u_{i+1}^n = u_{i-1}^n$  in the stencil (38) for  $i = N_x$  and obtain

$$u_i^{n+1} \approx -u_i^{n-1} + 2u_i^n + \left(\frac{\Delta x}{\Delta t}\right)^2 2q_i(u_{i-1}^n - u_i^n) + \Delta t^2 f_i^n$$

(We have used  $q_{i+\frac{1}{2}} + q_{i-\frac{1}{2}} \approx 2q_i$ .)

Alternative: assume  $dq/dx = 0$  (simpler).

# Implementation of variable coefficients

Assume  $c[i]$  holds  $c_i$  the spatial mesh points

```
for i in range(1, Nx):
    u[i] = - u_2[i] + 2*u_1[i] + \
            C2*(0.5*(q[i] + q[i+1])*(u_1[i+1] - u_1[i]) - \
                0.5*(q[i] + q[i-1])*(u_1[i] - u_1[i-1])) + \
            dt2*f(x[i], t[n])
```

Here:  $C2 = (dt/dx)**2$

Vectorized version:

```
u[1:-1] = - u_2[1:-1] + 2*u_1[1:-1] + \
            C2*(0.5*(q[1:-1] + q[2:])*(u_1[2:] - u_1[1:-1]) - \
                0.5*(q[1:-1] + q[:-2])*(u_1[1:-1] - u_1[:-2])) + \
            dt2*f(x[1:-1], t[n])
```

Neumann condition  $u_x = 0$ : same ideas as in 1D (modified stencil or ghost cells).

## A more general model PDE with variable coefficients

$$\varrho(x) \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left( q(x) \frac{\partial u}{\partial x} \right) + f(x, t) \quad (39)$$

A natural scheme is

$$[\varrho D_t D_t u = D_x \bar{q}^x D_x u + f]_i^n \quad (40)$$

Or

$$[D_t D_t u = \varrho^{-1} D_x \bar{q}^x D_x u + f]_i^n \quad (41)$$

No need to average  $\varrho$ , just sample at  $i$

# Generalization: damping

Why do waves die out?

- Damping (non-elastic effects, air resistance)
- 2D/3D: conservation of energy makes an amplitude reduction by  $1/\sqrt{r}$  (2D) or  $1/r$  (3D)

Simplest damping model (for physical behavior, see [demo](#)):

$$\frac{\partial^2 u}{\partial t^2} + b \frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} + f(x, t), \quad (42)$$

$b \geq 0$ : prescribed damping coefficient.

Discretization via centered differences to ensure  $\mathcal{O}(\Delta t^2)$  error:

$$[D_t D_t u + b D_{2t} u = c^2 D_x D_x u + f]_i^n \quad (43)$$

Need special formula for  $u_i^1$  + special stencil (or ghost cells) for Neumann conditions.

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver**
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

The program `wave1D_dn_vc.py` solves a fairly general 1D wave equation:

$$u_t = (c^2(x)u_x)_x + f(x, t), \quad x \in (0, L), \quad t \in (0, T] \quad (44)$$

$$u(x, 0) = I(x), \quad x \in [0, L] \quad (45)$$

$$u_t(x, 0) = V(t), \quad x \in [0, L] \quad (46)$$

$$u(0, t) = U_0(t) \text{ or } u_x(0, t) = 0, \quad t \in (0, T] \quad (47)$$

$$u(L, t) = U_L(t) \text{ or } u_x(L, t) = 0, \quad t \in (0, T] \quad (48)$$

Can be adapted to many needs.

The function `pulse` in `wave1D_dn_vc.py` offers four initial conditions:

- 1 a rectangular pulse ("plug")
- 2 a Gaussian function (gaussian)
- 3 a "cosine hat": one period of  $1 + \cos(\pi x)$ ,  $x \in [-1, 1]$
- 4 half a "cosine hat": half a period of  $\cos \pi x$ ,  $x \in [-\frac{1}{2}, \frac{1}{2}]$

Can locate the initial pulse at  $x = 0$  or in the middle

```
>>> import wave1D_dn_vc as w
>>> w.pulse(loc='left', pulse_tp='cosinehat', Nx=50, every_frame=10)
```



- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations**
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

Constant wave velocity  $c$ :

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u \text{ for } \mathbf{x} \in \Omega \subset \mathbb{R}^d, \ t \in (0, T] \quad (49)$$

Variable wave velocity:

$$\rho \frac{\partial^2 u}{\partial t^2} = \nabla \cdot (q \nabla u) + f \text{ for } \mathbf{x} \in \Omega \subset \mathbb{R}^d, \ t \in (0, T] \quad (50)$$

## Examples on wave equations written out in 2D/3D

3D, constant  $c$ :

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

2D, variable  $c$ :

$$\varrho(x, y) \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left( q(x, y) \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( q(x, y) \frac{\partial u}{\partial y} \right) + f(x, y, t) \quad (51)$$

Compact notation:

$$u_{tt} = c^2(u_{xx} + u_{yy} + u_{zz}) + f, \quad (52)$$

$$\varrho u_{tt} = (qu_x)_x + (qu_y)_y + (qu_z)_z + f \quad (53)$$

# Boundary and initial conditions

We need *one* boundary condition at *each point* on  $\partial\Omega$ :

- 1  $u$  is prescribed ( $u = 0$  or known incoming wave)
- 2  $\partial u / \partial n = \mathbf{n} \cdot \nabla u$  prescribed ( $= 0$ : reflecting boundary)
- 3 open boundary (radiation) condition:  $u_t + \mathbf{c} \cdot \nabla u = 0$  (let waves travel undisturbed out of the domain)

PDEs with *second-order* time derivative need *two* initial conditions:

- 1  $u = I,$
- 2  $u_t = V.$

- Mesh point:  $(x_i, y_j, z_k, t_n)$
- x direction:  $x_0 < x_1 < \cdots < x_{N_x}$
- y direction:  $y_0 < y_1 < \cdots < y_{N_y}$
- z direction:  $z_0 < z_1 < \cdots < z_{N_z}$
- $u_{i,j,k}^n \approx u_e(x_i, y_j, z_k, t_n)$

$$[D_t D_t u = c^2 (D_x D_x u + D_y D_y u) + f]_{i,j}^n,$$

Written out in detail:

$$\frac{u_{i,j}^{n+1} - 2u_{i,j}^n + u_{i,j}^{n-1}}{\Delta t^2} = c^2 \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + c^2 \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2} + f_{i,j}^n,$$

$u_{i,j}^{n-1}$  and  $u_{i,j}^n$  are known, solve for  $u_{i,j}^{n+1}$ :

$$u_{i,j}^{n+1} = 2u_{i,j}^n + u_{i,j}^{n-1} + c^2 \Delta t^2 [D_x D_x u + D_y D_y u]_{i,j}^n$$

## Special stencil for the first time step

- The stencil for  $u_{i,j}^1$  ( $n = 0$ ) involves  $u_{i,j}^{-1}$  which is outside the time mesh
- Remedy: use discretized  $u_t(x, 0) = V$  and the stencil for  $n = 0$  to develop a special stencil (as in the 1D case)

$$[D_{2t}u = V]_{i,j}^0 \Rightarrow u_{i,j}^{-1} = u_{i,j}^1 - 2\Delta t V_{i,j}$$

$$u_{i,j}^{n+1} = u_{i,j}^n - 2\Delta V_{i,j} + \frac{1}{2}c^2\Delta t^2[D_x D_x u + D_y D_y u]_{i,j}^n$$

## Variable coefficients (1)

3D wave equation:

$$\varrho u_{tt} = (qu_x)_x + (qu_y)_y + (qu_z)_z + f(x, y, z, t)$$

Just apply the 1D discretization for each term:

$$[\varrho D_t D_t u = (D_x \bar{q}^x D_x u + D_y \bar{q}^y D_y u + D_z \bar{q}^z D_z u) + f]_{i,j,k}^n \quad (54)$$

Need special formula for  $u_{i,j,k}^1$  (use  $[D_{2t} u = V]^0$  and stencil for  $n = 0$ ).



## Variable coefficients (2)

Written out:

$$\begin{aligned}u_{i,j,k}^{n+1} &= -u_{i,j,k}^{n-1} + 2u_{i,j,k}^n + \\&= \frac{1}{\varrho_{i,j,k}} \frac{1}{\Delta x^2} \left( \frac{1}{2} (q_{i,j,k} + q_{i+1,j,k}) (u_{i+1,j,k}^n - u_{i,j,k}^n) - \right. \\&\quad \left. \frac{1}{2} (q_{i-1,j,k} + q_{i,j,k}) (u_{i,j,k}^n - u_{i-1,j,k}^n) \right) + \\&= \frac{1}{\varrho_{i,j,k}} \frac{1}{\Delta x^2} \left( \frac{1}{2} (q_{i,j,k} + q_{i,j+1,k}) (u_{i,j+1,k}^n - u_{i,j,k}^n) - \right. \\&\quad \left. \frac{1}{2} (q_{i,j-1,k} + q_{i,j,k}) (u_{i,j,k}^n - u_{i,j-1,k}^n) \right) + \\&= \frac{1}{\varrho_{i,j,k}} \frac{1}{\Delta x^2} \left( \frac{1}{2} (q_{i,j,k} + q_{i,j,k+1}) (u_{i,j,k+1}^n - u_{i,j,k}^n) - \right. \\&\quad \left. \frac{1}{2} (q_{i,j,k-1} + q_{i,j,k}) (u_{i,j,k}^n - u_{i,j,k-1}^n) \right) + \\&\quad + \Delta t^2 f_{i,j,k}^n\end{aligned}$$

## Neumann boundary condition in 2D

Use ideas from 1D! Example:  $\frac{\partial u}{\partial n}$  at  $y = 0$ ,  $\frac{\partial u}{\partial n} = -\frac{\partial u}{\partial y}$

Boundary condition discretization:

$$[-D_{2y}u = 0]_{i,0}^n \Rightarrow \frac{u_{i,1}^n - u_{i,-1}^n}{2\Delta y} = 0, \quad i \in \mathcal{I}_x$$

Insert  $u_{i,-1}^n = u_{i,1}^n$  in the stencil for  $u_{i,j=0}^{n+1}$  to obtain a modified stencil on the boundary.

Pattern: use interior stencil also on the boundary, but replace  $j - 1$  by  $j + 1$

Alternative: use ghost cells and ghost values

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems**
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

$$u_t = c^2(u_{xx} + u_{yy}) + f(x, y, t), \quad (x, y) \in \Omega, \quad t \in (0, T] \quad (55)$$

$$u(x, y, 0) = I(x, y), \quad (x, y) \in \Omega \quad (56)$$

$$u_t(x, y, 0) = V(x, y), \quad (x, y) \in \Omega \quad (57)$$

$$u = 0, \quad (x, y) \in \partial\Omega, \quad t \in (0, T] \quad (58)$$

$$\Omega = [0, L_x] \times [0, L_y]$$

Discretization:

$$[D_t D_t u = c^2(D_x D_x u + D_y D_y u) + f]_{i,j}^n,$$

- ➊ Set initial condition  $u_{i,j}^0 = I(x_i, y_j)$
- ➋ Compute  $u_{i,j}^1 = \dots$  for  $i \in \mathcal{I}_x^i$  and  $j \in \mathcal{I}_y^i$
- ➌ Set  $u_{i,j}^1 = 0$  for the boundaries  $i = 0, N_x, j = 0, N_y$
- ➍ For  $n = 1, 2, \dots, N_t$ :
  - ➊ Find  $u_{i,j}^{n+1} = \dots$  for  $i \in \mathcal{I}_x^i$  and  $j \in \mathcal{I}_y^i$
  - ➋ Set  $u_{i,j}^{n+1} = 0$  for the boundaries  $i = 0, N_x, j = 0, N_y$

# Scalar computations: mesh

Program: `wave2D_u0.py`

```
def solver(I, V, f, c, Lx, Ly, Nx, Ny, dt, T,  
           user_action=None, version='scalar'):
```

Mesh:

```
x = linspace(0, Lx, Nx+1)           # mesh points in x dir  
y = linspace(0, Ly, Ny+1)           # mesh points in y dir  
dx = x[1] - x[0]  
dy = y[1] - y[0]  
Nt = int(round(T/float(dt)))  
t = linspace(0, N*dt, N+1)           # mesh points in time  
Cx2 = (c*dt/dx)**2; Cy2 = (c*dt/dy)**2 # help variables  
dt2 = dt**2
```

## Scalar computations: arrays

Store  $u_{i,j}^{n+1}$ ,  $u_{i,j}^n$ , and  $u_{i,j}^{n-1}$  in three two-dimensional arrays:

```
u    = zeros((Nx+1,Ny+1))    # solution array
u_1  = zeros((Nx+1,Ny+1))    # solution at t-dt
u_2  = zeros((Nx+1,Ny+1))    # solution at t-2*dt
```

$u_{i,j}^{n+1}$  corresponds to `u[i,j]`, etc.

## Scalar computations: initial condition

```
Ix = range(0, u.shape[0])
Iy = range(0, u.shape[1])
It = range(0, t.shape[0])

for i in Ix:
    for j in Iy:
        u_1[i,j] = I(x[i], y[j])

if user_action is not None:
    user_action(u_1, x, xv, y, yv, t, 0)
```

Arguments xv and yv: for vectorized computations



# Scalar computations: primary stencil

```
def advance_scalar(u, u_1, u_2, f, x, y, t, n, Cx2, Cy2, dt2,
                  V=None, step1=False):
    Ix = range(0, u.shape[0]);  Iy = range(0, u.shape[1])
    if step1:
        dt = sqrt(dt2)  # save
        Cx2 = 0.5*Cx2;  Cy2 = 0.5*Cy2; dt2 = 0.5*dt2  # redefine
        D1 = 1;  D2 = 0
    else:
        D1 = 2;  D2 = 1
    for i in Ix[1:-1]:
        for j in Iy[1:-1]:
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = D1*u_1[i,j] - D2*u_2[i,j] + \
                    Cx2*u_xx + Cy2*u_yy + dt2*f(x[i], y[j], t[n])
            if step1:
                u[i,j] += dt*V(x[i], y[j])
    # Boundary condition u=0
    j = Iy[0]
    for i in Ix: u[i,j] = 0
    j = Iy[-1]
    for i in Ix: u[i,j] = 0
    i = Ix[0]
    for j in Iy: u[i,j] = 0
    i = Ix[-1]
    for j in Iy: u[i,j] = 0
    return u
```

# Vectorized computations: mesh coordinates

Mesh with  $30 \times 30$  cells: vectorization reduces the CPU time by a factor of 70 (!).

Need special coordinate arrays  $xv$  and  $yv$  such that  $I(x, y)$  and  $f(x, y, t)$  can be vectorized:

```
from numpy import newaxis
xv = x[:,newaxis]
yv = y[newaxis,:]

u_1[:,:] = I(xv, yv)
f_a[:,:] = f(xv, yv, t)
```

# Vectorized computations: stencil

```
def advance_vectorized(u, u_1, u_2, f_a, Cx2, Cy2, dt2,
                      V=None, step1=False):
    if step1:
        dt = sqrt(dt2)    # save
        Cx2 = 0.5*Cx2;   Cy2 = 0.5*Cy2; dt2 = 0.5*dt2    # redefine
        D1 = 1;   D2 = 0
    else:
        D1 = 2;   D2 = 1
    u_xx = u_1[:-2,1:-1] - 2*u_1[1:-1,1:-1] + u_1[2:,1:-1]
    u_yy = u_1[1:-1,:-2] - 2*u_1[1:-1,1:-1] + u_1[1:-1,2:]
    u[1:-1,1:-1] = D1*u_1[1:-1,1:-1] - D2*u_2[1:-1,1:-1] + \
        Cx2*u_xx + Cy2*u_yy + dt2*f_a[1:-1,1:-1]
    if step1:
        u[1:-1,1:-1] += dt*V[1:-1, 1:-1]
    # Boundary condition u=0
    j = 0
    u[:,j] = 0
    j = u.shape[1]-1
    u[:,j] = 0
    i = 0
    u[i,:] = 0
    i = u.shape[0]-1
    u[i,:] = 0
    return u
```

## Verification: quadratic solution (1)

Manufactured solution:

$$u_e(x, y, t) = x(L_x - x)y(L_y - y)(1 + \frac{1}{2}t) \quad (59)$$

Requires  $f = 2c^2(1 + \frac{1}{2}t)(y(L_y - y) + x(L_x - x))$ .

This  $u_e$  is ideal because it also solves the discrete equations!

## Verification: quadratic solution (2)

- $[D_t D_t 1]^n = 0$
- $[D_t D_t t]^n = 0$
- $[D_t D_t t^2] = 2$
- $D_t D_t$  is a linear operator:  
 $[D_t D_t (au + bv)]^n = a[D_t D_t u]^n + b[D_t D_t v]^n$

$$\begin{aligned}[D_x D_x u_e]_{i,j}^n &= [y(L_y - y)(1 + \frac{1}{2}t) D_x D_x x(L_x - x)]_{i,j}^n \\ &= y_j(L_y - y_j)(1 + \frac{1}{2}t_n)2\end{aligned}$$

- Similar calculations for  $[D_y D_y u_e]_{i,j}^n$  and  $[D_t D_t u_e]_{i,j}^n$  terms
- Must also check the equation for  $u_{i,j}^1$

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython**
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

- Vectorization: 5-10 times slower than pure C or Fortran code
- Cython: extension of Python for translating functions to C
- Principle: declare variables with type

# Declaring variables and annotating the code

Pure Python code:

```
def advance_scalar(u, u_1, u_2, f, x, y, t,
                  n, Cx2, Cy2, dt2, D1=2, D2=1):
    Ix = range(0, u.shape[0]); Iy = range(0, u.shape[1])
    for i in Ix[1:-1]:
        for j in Iy[1:-1]:
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = D1*u_1[i,j] - D2*u_2[i,j] + \
                Cx2*u_xx + Cy2*u_yy + dt2*f(x[i], y[j], t[n])
```

- Copy this function and put it in a file with .pyx extension.
- Add type of variables:
  - `function(a, b) → cpdef function(int a, double b)`
  - `v = 1.2 → cdef double v = 1.2`
  - Array declaration:  
`np.ndarray[np.float64_t, ndim=2, mode='c'] u`



# Cython version of the functions

```
import numpy as np
cimport numpy as np
cimport cython
ctypedef np.float64_t DT      # data type

@cython.boundscheck(False)    # turn off array bounds check
@cython.wraparound(False)    # turn off negative indices (u[-1,-1])
cpdef advance(
    np.ndarray[DT, ndim=2, mode='c'] u,
    np.ndarray[DT, ndim=2, mode='c'] u_1,
    np.ndarray[DT, ndim=2, mode='c'] u_2,
    np.ndarray[DT, ndim=2, mode='c'] f,
    double Cx2, double Cy2, double dt2):

    cdef int Nx, Ny, i, j
    cdef double u_xx, u_yy
    Nx = u.shape[0]-1
    Ny = u.shape[1]-1
    for i in xrange(1, Nx):
        for j in xrange(1, Ny):
            u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
            u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
            u[i,j] = 2*u_1[i,j] - u_2[i,j] + \
                Cx2*u_xx + Cy2*u_yy + dt2*f[i,j]
```

Note: from now in we skip the code for setting boundary values

# Visual inspection of the C translation

See how effective Cython can translate this code to C:

```
Terminal> cython -a wave2D_u0_loop_cy.pyx
```

Load `wave2D_u0_loop_cy.html` in a browser (white: pure C, yellow: still Python):

Raw output: [wave2D\\_u0\\_loop\\_cy.c](#)

```
1: import numpy as np
2: cimport numpy as np
3: cimport cython
4: ctypedef np.float64_t DT    # data type
5:
6: @cython.boundscheck(False)  # turn off array bounds check
7: @cython.wraparound(False)   # turn off negative indices (u[-1,-1])
8: cdef advance(
9:     np.ndarray[DT, ndim=2, mode='c'] u,
10:     np.ndarray[DT, ndim=2, mode='c'] u_1,
11:     np.ndarray[DT, ndim=2, mode='c'] u_2,
12:     np.ndarray[DT, ndim=2, mode='c'] f,
13:     double Cx2, double Cy2, double dt2):
14:
15:     cdef int Ix_start = 0
16:     cdef int Iy_start = 0
17:     cdef int Ix_end = u.shape[0]-1
18:     cdef int Iy_end = u.shape[1]-1
19:     cdef int i, j
20:     cdef double u_xx, u_yy
21:
22:     for i in range(Ix_start+1, Ix_end):
23:         for j in range(Iy_start+1, Iy_end):
24:             u_xx = u_1[i-1,j] - 2*u_1[i,j] + u_1[i+1,j]
25:             u_yy = u_1[i,j-1] - 2*u_1[i,j] + u_1[i,j+1]
26:             u[i,j] = 2*u_1[i,j] - u_2[i,j] + \
27:                 Cx2*u_xx + Cy2*u_yy + dt2*f[i,j]
28:
29:     # Boundary condition u=0
30:     j = Iy_start
31:     for i in range(Ix_start, Ix_end+1): u[i,j] = 0
32:     j = Iy_end
33:     for i in range(Ix_start, Ix_end+1): u[i,j] = 0
34:     i = Ix_start
35:     for j in range(Iy_start, Iy_end+1): u[i,j] = 0
36:     i = Iy_end
37:     for j in range(Iy_start, Iy_end+1): u[i,j] = 0
38:
39:     return u
```

Can click on `wave2D_u0_loop_cy.c` to see the generated C code...

# Building the extension module

- Cython code must be translated to C
- C code must be compiled
- Compiled C code must be linked to Python C libraries
- Result: *C extension module* (.so file) that can be loaded as a standard Python module
- Use a `setup.py` script to build the extension module

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

cymodule = 'wave2D_u0_loop_cy'
setup(
    name=cymodule,
    ext_modules=[Extension(cymodule, [cymodule + '.pyx'],)],
    cmdclass={'build_ext': build_ext},
)
```

```
Terminal> python setup.py build_ext --inplace
```

# Calling the Cython function from Python

```
import wave2D_u0_loop_cy
advance = wave2D_u0_loop_cy.advance
...
for n in It[1:-1:]:                # time loop
    f_a[:, :] = f(xv, yv, t[n])    # precompute, size as u
    u = advance(u, u_1, u_2, f_a, x, y, t, Cx2, Cy2, dt2)
```

Efficiency:

- $120 \times 120$  cells in space:
  - Pure Python: 1370 CPU time units
  - Vectorized numpy: 5.5
  - Cython: 1
- $60 \times 60$  cells in space:
  - Pure Python: 1000 CPU time units
  - Vectorized numpy: 6
  - Cython: 1

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran**
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

- Write the advance function in pure Fortran
- Use f2py to generate C code for calling Fortran from Python
- Full manual control of the translation to Fortran

# The Fortran subroutine

```
subroutine advance(u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny)
integer Nx, Ny
real*8 u(0:Nx,0:Ny), u_1(0:Nx,0:Ny), u_2(0:Nx,0:Ny)
real*8 f(0:Nx, 0:Ny), Cx2, Cy2, dt2
integer i, j
Cf2py intent(in, out) u

C    Scheme at interior points
do j = 1, Ny-1
  do i = 1, Nx-1
    u(i,j) = 2*u_1(i,j) - u_2(i,j) +
&    Cx2*(u_1(i-1,j) - 2*u_1(i,j) + u_1(i+1,j)) +
&    Cy2*(u_1(i,j-1) - 2*u_1(i,j) + u_1(i,j+1)) +
&    dt2*f(i,j)
  end do
end do
```

Note: Cf2py comment declares u as input argument and return value back to Python

# Building the Fortran module with f2py

```
Terminal> f2py -m wave2D_u0_loop_f77 -h wave2D_u0_loop_f77.pyf \  
--overwrite-signature wave2D_u0_loop_f77.f  
Terminal> f2py -c wave2D_u0_loop_f77.pyf --build-dir build_f77 \  
-DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_f77.f
```

f2py changes the argument list (!)

```
>>> import wave2D_u0_loop_f77  
>>> print wave2D_u0_loop_f77.__doc__  
This module 'wave2D_u0_loop_f77' is auto-generated with f2py....  
Functions:  
    u = advance(u,u_1,u_2,f,cx2,cy2,dt2,  
               nx=(shape(u,0)-1),ny=(shape(u,1)-1))
```

- Array limits have default values
- Examine doc strings from f2py!



# How to avoid array copying

- Two-dimensional arrays are stored row by row in Python and C
- Two-dimensional arrays are stored column by column in Fortran
- f2py takes a copy of a numpy (C) array and transposes it when calling Fortran
- Such copies are time and memory consuming
- Remedy: declare numpy arrays with Fortran storage

```
order = 'Fortran' if version == 'f77' else 'C'
u      = zeros((Nx+1,Ny+1), order=order)
u_1    = zeros((Nx+1,Ny+1), order=order)
u_2    = zeros((Nx+1,Ny+1), order=order)
```

Option `-DF2PY_REPORT_ON_ARRAY_COPY=1` makes f2py write out array copying:

```
Terminal> f2py -c wave2D_u0_loop_f77.pyf --build-dir build_f77 \
           -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_f77.f
```

# Efficiency of translating to Fortran

- Same efficiency (in this example) as Cython and C
- About 5 times faster than vectorized `numpy` code
- $> 1000$  faster than pure Python code

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython**
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations

- Write the advance function in pure C
- Use Cython to generate C code for calling C from Python
- Full manual control of the translation to C

# The C code

- numpy arrays transferred to C are one-dimensional in C
- Need to translate  $[i,j]$  indices to single indices

```
/* Translate (i,j) index to single array index */
#define idx(i,j) (i)*(Ny+1) + j

void advance(double* u, double* u_1, double* u_2, double* f,
             double Cx2, double Cy2, double dt2,
             int Nx, int Ny)
{
    int i, j;
    /* Scheme at interior points */
    for (i=1; i<=Nx-1; i++) {
        for (j=1; j<=Ny-1; j++) {
            u[idx(i,j)] = 2*u_1[idx(i,j)] - u_2[idx(i,j)] +
                Cx2*(u_1[idx(i-1,j)] - 2*u_1[idx(i,j)] + u_1[idx(i+1,j)]) +
                Cy2*(u_1[idx(i,j-1)] - 2*u_1[idx(i,j)] + u_1[idx(i,j+1)]) +
                dt2*f[idx(i,j)];
        }
    }
}
```

# The Cython interface file

```
import numpy as np
cimport numpy as np
cimport cython

cdef extern from "wave2D_u0_loop_c.h":
    void advance(double* u, double* u_1, double* u_2, double* f,
                 double Cx2, double Cy2, double dt2,
                 int Nx, int Ny)

@cython.boundscheck(False)
@cython.wraparound(False)
def advance_cwrap(
    np.ndarray[double, ndim=2, mode='c'] u,
    np.ndarray[double, ndim=2, mode='c'] u_1,
    np.ndarray[double, ndim=2, mode='c'] u_2,
    np.ndarray[double, ndim=2, mode='c'] f,
    double Cx2, double Cy2, double dt2):
    advance(&u[0,0], &u_1[0,0], &u_2[0,0], &f[0,0],
           Cx2, Cy2, dt2,
           u.shape[0]-1, u.shape[1]-1)
    return u
```

# Building the extension module

Compile and link the extension module with a setup.py file:

```
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

sources = ['wave2D_u0_loop_c.c', 'wave2D_u0_loop_c_cy.pyx']
module = 'wave2D_u0_loop_c_cy'
setup(
    name=module,
    ext_modules=[Extension(module, sources,
                           libraries=[], # C libs to link with
                           )],
    cmdclass={'build_ext': build_ext},
)
```

```
Terminal> python setup.py build_ext --inplace
```

In Python:

```
import wave2D_u0_loop_c_cy
advance = wave2D_u0_loop_c_cy.advance_cwrap
...
f_a[:, :] = f(xv, yv, t[n])
u = advance(u, u_1, u_2, f_a, Cx2, Cy2, dt2)
```

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py**
- 14 Analysis of the difference equations



- Write the advance function in pure C
- Use f2py to generate C code for calling C from Python
- Full manual control of the translation to C

# The C code and the Fortran interface file

- Write the C function advance as before
- Write a Fortran 90 module defining the signature of the advance function
- Or: write a Fortran 77 function defining the signature and let f2py generate the Fortran 90 module

Fortran 77 signature (note `intent(c)`):

```
subroutine advance(u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny)
Cf2py intent(c) advance
integer Nx, Ny, N
real*8 u(0:Nx,0:Ny), u_1(0:Nx,0:Ny), u_2(0:Nx,0:Ny)
real*8 f(0:Nx, 0:Ny), Cx2, Cy2, dt2
Cf2py intent(in, out) u
Cf2py intent(c) u, u_1, u_2, f, Cx2, Cy2, dt2, Nx, Ny
return
end
```

# Building the extension module

Generate Fortran 90 module (wave2D\_u0\_loop\_c\_f2py.pyf):

```
Terminal> f2py -m wave2D_u0_loop_c_f2py \  
            -h wave2D_u0_loop_c_f2py.pyf --overwrite-signature \  
            wave2D_u0_loop_c_f2py_signature.f
```

The compile and build step must list the C files:

```
Terminal> f2py -c wave2D_u0_loop_c_f2py.pyf \  
            --build-dir tmp_build_c \  
            -DF2PY_REPORT_ON_ARRAY_COPY=1 wave2D_u0_loop_c.c
```

# Migrating loops to C++ via f2py

- C++ can be used as an alternative to C
- C++ code often applies sophisticated arrays
- Challenge: translate from numpy C arrays to C++ array classes
- Can use SWIG to make C++ classes available as Python classes
- Easier (and more efficient):
  - Make C API to the C++ code
  - Wrap C API with f2py
  - Send numpy arrays to C API and let C translate numpy arrays into C++ array classes

- 1 Finite difference methods for waves on a string
- 2 Verification
- 3 Implementation
  - Making a solver function (3)
- 4 Vectorization
- 5 Generalization: reflecting boundaries
- 6 Generalization: variable wave velocity
- 7 Building a general 1D wave equation solver
- 8 Finite difference methods for 2D and 3D wave equations
- 9 Implementation of 2D/3D problems
- 10 Migrating loops to Cython
- 11 Migrating loops to Fortran
- 12 Migrating loops to C via Cython
- 13 Migrating loops to C via f2py
- 14 Analysis of the difference equations**

# Properties of the solution of the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Solutions:

$$u(x, t) = g_R(x - ct) + g_L(x + ct), \quad (60)$$

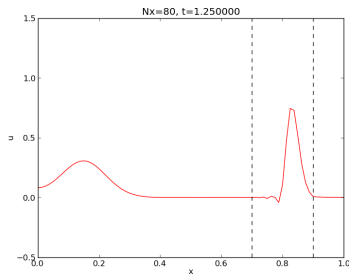
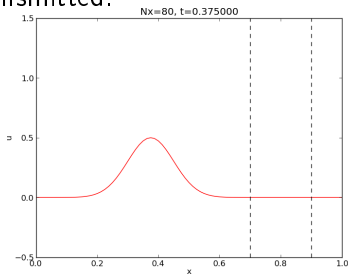
If  $u(x, 0) = l(x)$  and  $u_t(x, 0) = 0$ :

$$u(x, t) = \frac{1}{2}l(x - ct) + \frac{1}{2}l(x + ct) \quad (61)$$

Two waves: one traveling to the right and one to the left

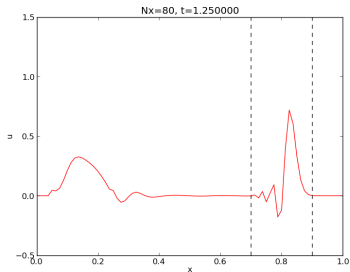
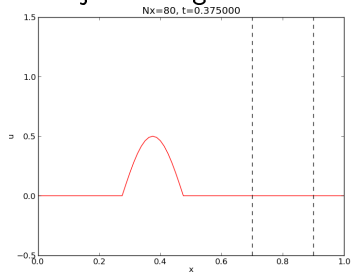
# Effect of variable wave velocity

A wave propagates perfectly ( $C = 1$ ) and hits a medium with  $1/4$  of the wave velocity. A part of the wave is reflected and the rest is transmitted.



# What happens here?

We have just changed the initial condition...





# Representation of waves as sum of sine/cosine waves

Build  $I(x)$  of wave components  $e^{ikx} = \cos kx + i \sin kx$ :

$$I(x) \approx \sum_{k \in K} b_k e^{ikx} \quad (62)$$

- $k$  is the frequency of a component ( $\lambda = 2\pi/k$  corresponding wave length)
- $K$  is some set of all  $k$  needed to approximate  $I(x)$  well
- $b_k$  must be computed (Fourier coefficients)

Since  $u(x, t) = \frac{1}{2}I(x - ct) + \frac{1}{2}I(x + ct)$ :

$$u(x, t) = \frac{1}{2} \sum_{k \in K} b_k e^{ik(x-ct)} + \frac{1}{2} \sum_{k \in K} b_k e^{ik(x+ct)} \quad (63)$$

Our interest: one component  $e^{i(kx - \omega t)}$ ,  $\omega = kc$

A similar discrete  $u_q^n = e^{i(kx_q - \tilde{\omega}t_n)}$  solves

$$[D_t D_t u = c^2 D_x D_x u]_q^n \quad (64)$$

Note: different frequency  $\tilde{\omega} \neq \omega$

- How accurate is  $\tilde{\omega}$  compared to  $\omega$ ?
- What about the wave amplitude?

$$[D_t D_t e^{i\omega t}]^n = -\frac{4}{\Delta t^2} \sin^2 \left( \frac{\omega \Delta t}{2} \right) e^{i\omega n \Delta t}$$

By  $\omega \rightarrow k$ ,  $t \rightarrow x$ ,  $n \rightarrow q$ ) it follows that

$$[D_x D_x e^{ikx}]_q = -\frac{4}{\Delta x^2} \sin^2 \left( \frac{k \Delta x}{2} \right) e^{ikq \Delta x}$$

# Numerical wave propagation (1)

Inserting a basic wave component  $u = e^{i(kx_q - \tilde{\omega}t_n)}$  in the scheme (64) requires computation of

$$\begin{aligned} [D_t D_t e^{ikx} e^{-i\tilde{\omega}t}]_q^n &= [D_t D_t e^{-i\tilde{\omega}t}]^n e^{ikq\Delta x} \\ &= -\frac{4}{\Delta t^2} \sin^2\left(\frac{\tilde{\omega}\Delta t}{2}\right) e^{-i\tilde{\omega}n\Delta t} e^{ikq\Delta x} \end{aligned} \quad (65)$$

$$\begin{aligned} [D_x D_x e^{ikx} e^{-i\tilde{\omega}t}]_q^n &= [D_x D_x e^{ikx}]_q e^{-i\tilde{\omega}n\Delta t} \\ &= -\frac{4}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right) e^{ikq\Delta x} e^{-i\tilde{\omega}n\Delta t} \end{aligned} \quad (66)$$

## Numerical wave propagation (2)

The complete scheme,

$$[D_t D_t e^{ikx} e^{-i\tilde{\omega}t} = c^2 D_x D_x e^{ikx} e^{-i\tilde{\omega}t}]_q^n$$

leads to an equation for  $\tilde{\omega}$ :

$$\sin^2 \left( \frac{\tilde{\omega} \Delta t}{2} \right) = C^2 \sin^2 \left( \frac{k \Delta x}{2} \right), \quad (67)$$

where  $C = \frac{c \Delta t}{\Delta x}$  is the Courant number

Taking the square root of (67):

$$\sin\left(\frac{\tilde{\omega}\Delta t}{2}\right) = C \sin\left(\frac{k\Delta x}{2}\right), \quad (68)$$

- Exact  $\omega$  is real
- Look for a real solution  $\tilde{\omega}$  of (68)
- Then the sine functions are in  $[-1, 1]$
- Lef-hand side in  $[-1, 1]$  requires  $C \leq 1$

Stability criterion

$$C = \frac{c\Delta t}{\Delta x} \leq 1 \quad (69)$$

## Why $C \leq 1$ is a stability criterion

Assume  $C > 1$ . Then

$$\underbrace{\sin\left(\frac{\tilde{\omega}\Delta t}{2}\right)} > 1 = C \sin\left(\frac{k\Delta x}{2}\right)$$

- $|\sin x| > 1$  implies complex  $x$
- Here: complex  $\tilde{\omega} = \tilde{\omega}_r \pm i\tilde{\omega}_i$
- One  $\tilde{\omega}_i < 0$  gives  $\exp(i \cdot i\tilde{\omega}_i) = \exp(\tilde{\omega}_i)$  and exponential growth

# Numerical dispersion relation

- How close is  $\tilde{\omega}$  to  $\omega$ ?
- Can solve for an explicit formula for  $\tilde{\omega}$

$$\tilde{\omega} = \frac{2}{\Delta t} \sin^{-1} \left( C \sin \left( \frac{k \Delta x}{2} \right) \right) \quad (70)$$

- $\omega = kc$  is the *analytical dispersion relation*
- $\tilde{\omega} = \tilde{\omega}(k, c, \Delta x, \Delta t)$  is the *numerical dispersion relation*
- Speed of waves:  $c = \omega/k$ ,  $\tilde{c} = \tilde{\omega}/k$
- The numerical wave component has a wrong, mesh-dependent speed



## The special case $C = 1$

- For  $C = 1$ ,  $\tilde{\omega} = \omega$
- The numerical solution is exact (at the mesh points)!
- The only requirement is constant  $c$

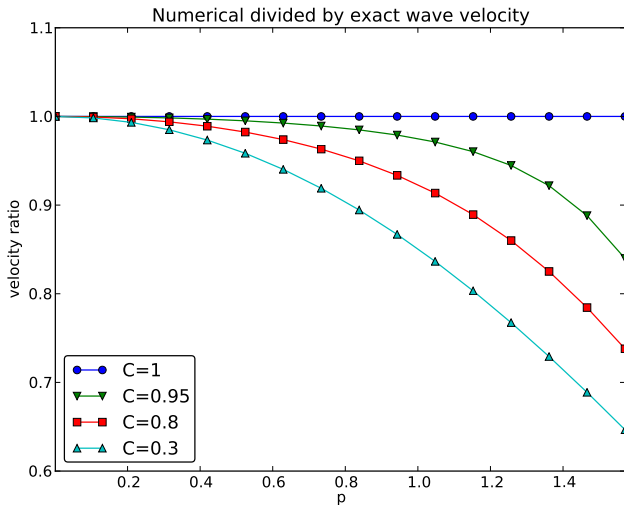
# Computing the error in wave velocity

- Introduce  $p = k\Delta x/2$
- $p$  measures no of mesh points in space per wave length in space
- Study error in wave velocity through  $\tilde{c}/c$  as function of  $p$

$$r(C, p) = \frac{\tilde{c}}{c} = \frac{1}{Cp} \sin^{-1}(C \sin p), \quad C \in (0, 1], \quad p \in (0, \pi/2]$$

# Visualizing the error in wave velocity

```
def r(C, p):  
    return 2/(C*p)*asin(C*sin(p))
```



Note: the shortest waves have the largest error, and short waves

# Taylor expanding the error in wave velocity

For small  $p$ , Taylor expand  $\tilde{\omega}$  as polynomial in  $p$ :

```
>>> C, p = symbols('C p')
>>> rs = r(C, p).series(p, 0, 7)
>>> print rs
1 - p**2/6 + p**4/120 - p**6/5040 + C**2*p**2/6 -
C**2*p**4/12 + 13*C**2*p**6/720 + 3*C**4*p**4/40 -
C**4*p**6/16 + 5*C**6*p**6/112 + O(p**7)

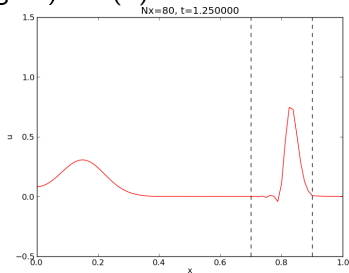
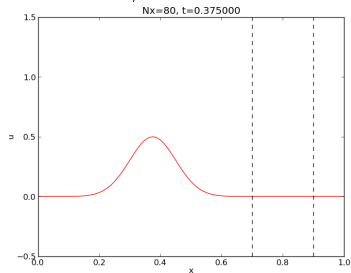
>>> # Factorize each term and drop the remainder O(...) term
>>> rs_factored = [factor(term) for term in rs.lseries(p)]
>>> rs_factored = sum(rs_factored)
>>> print rs_factored
p**6*(C - 1)*(C + 1)*(225*C**4 - 90*C**2 + 1)/5040 +
p**4*(C - 1)*(C + 1)*(3*C - 1)*(3*C + 1)/120 +
p**2*(C - 1)*(C + 1)/6 + 1
```

Leading error term is  $\frac{1}{6}(C^2 - 1)p^2$  or

$$\frac{1}{6} \left( \frac{k\Delta x}{2} \right)^2 (C^2 - 1) = \frac{k^2}{24} (c^2 \Delta t^2 - \Delta x^2) = \mathcal{O}(\Delta t^2, \Delta x^2) \quad (71)$$

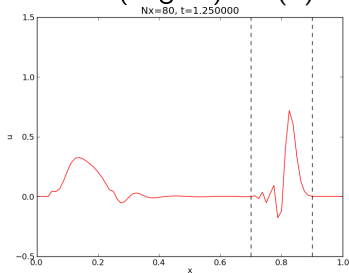
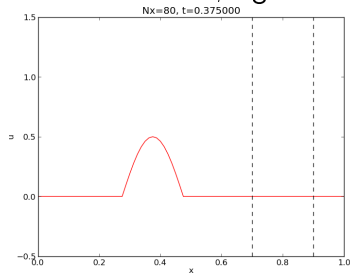
# Example on effect of wrong wave velocity (1)

Smooth wave, few short waves (large  $k$ ) in  $I(x)$ :



# Example on effect of wrong wave velocity (1)

Not so smooth wave, significant short waves (large  $k$ ) in  $I(x)$ :



## Extending the analysis to 2D (and 3D)

$$u(x, y, t) = g(k_x x + k_y y - \omega t)$$

is a typically solution of

$$u_{tt} = c^2(u_{xx} + u_{yy})$$

Can build solutions by adding complex Fourier components of the form

$$e^{i(k_x x + k_y y - \omega t)}$$

$$[D_t D_t u = c^2(D_x D_x u + D_y D_y u)]_{q,r}^n \quad (72)$$

This equation admits a Fourier component

$$u_{q,r}^n = e^{i(k_x q \Delta x + k_y r \Delta y - \tilde{\omega} n \Delta t)} \quad (73)$$

Inserting the expression and using formulas from the 1D analysis:

$$\sin^2 \left( \frac{\tilde{\omega} \Delta t}{2} \right) = C_x^2 \sin^2 p_x + C_y^2 \sin^2 p_y, \quad (74)$$

where

$$C_x = \frac{c^2 \Delta t^2}{\Delta x^2}, \quad C_y = \frac{c^2 \Delta t^2}{\Delta y^2}, \quad p_x = \frac{k_x \Delta x}{2}, \quad p_y = \frac{k_y \Delta y}{2}$$



Real-valued  $\tilde{\omega}$  requires

$$C_x^2 + C_y^2 \leq 1 \quad (75)$$

or

$$\Delta t \leq \frac{1}{c} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1/2} \quad (76)$$

$$\Delta t \leq \frac{1}{c} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-1/2} \quad (77)$$

For  $c^2 = c^2(\mathbf{x})$  we must use the worst-case value  $\bar{c} = \sqrt{\max_{\mathbf{x} \in \Omega} c^2(\mathbf{x})}$  and a safety factor  $\beta \leq 1$ :

$$\Delta t \leq \beta \frac{1}{\bar{c}} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{-1/2} \quad (78)$$

## Numerical dispersion relation in 2D (1)

$$\tilde{\omega} = \frac{2}{\Delta t} \sin^{-1} \left( (C_x^2 \sin^2 p_x + C_y^2 \sin^2 p_y)^{\frac{1}{2}} \right)$$

For visualization, introduce  $\theta$ :

$$k_x = k \sin \theta, \quad k_y = k \cos \theta, \quad p_x = \frac{1}{2}kh \cos \theta, \quad p_y = \frac{1}{2}kh \sin \theta$$

Also:  $\Delta x = \Delta y = h$ . Then  $C_x = C_y = c\Delta t/h \equiv C$ .

Now  $\tilde{\omega}$  depends on

- $C$  reflecting the number cells a wave is displaced during a time step
- $kh$  reflecting the number of cells per wave length in space
- $\theta$  expressing the direction of the wave

## Numerical dispersion relation in 2D (2)

$$\frac{\tilde{c}}{c} = \frac{1}{Ckh} \sin^{-1} \left( C \left( \sin^2\left(\frac{1}{2}kh \cos \theta\right) + \sin^2\left(\frac{1}{2}kh \sin \theta\right) \right)^{\frac{1}{2}} \right)$$

Can make color contour plots of  $1 - \tilde{c}/c$  in *polar coordinates* with  $\theta$  as the angular coordinate and  $kh$  as the radial coordinate.

# Numerical dispersion relation in 2D (3)

